東京大学グローバルCOEプログラム　機械システム・イノベーション国際拠点

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What Can We Learn from Current Molecular Dynamics Simulations of Nanotube Growth?

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要旨

We present the results of nonequilibrium molecular dynamics(MD) simulations of catalytic and non-catalytic carbon nanotube nucleation and growth. The focus is in particular on the delicate balance of defect formation and healing, as viewed from the perspective of parameters such as feedstock addition rates, temperature, carbon concentrations which are often far from experiment due to computational constraints. Thus, the significance of the findings from MD simulations are discussed in relation to available insights from experiment on one hand, and to "static" theoretical studies of growth that are guided by Thermodynamics on the other.

主催：　東京大学グローバルCOEプログラム「機械システム・イノベーション国際拠点」
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